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A simple approach to prove the addition theorem for regular solid harmonics

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Abstract : We present a simple approach to express $r_{12}^L Y_{LM}(\hat{r}_{12})$, with $\boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2$ as a sum of the products of $r_1^{l_1} Y_{l_1 m_1}(\hat{r}_1)$ and $r_2^{l_2} Y_{l_2 m_2}(\hat{r}_2)$.

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Many problems of theoretical physics call for the representation of the regular solid harmonics $r_{12}^L Y_{LM}(\hat{r}_{12})$ in terms of the regular solid harmonics of the vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ where $\boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. Such a representation is generally known as the addition theorem for regular solid harmonics. There exists quite a number of approaches [1,10] to derive this addition theorem. Among them Caola's [10] approach is the simplest one. However, his derivation is based on an identity due to Hobson [11] which is not so well known. In this note, we present an alternative derivation using only the familiar results.

We start with the well known expansion

$$e^{i\boldsymbol{K}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)} = 4\pi\sum_{lm} i^l j_l(Kr_{12})\, Y_{lm}^*(\hat{K})\, Y_{lm}(\hat{r}_{12}). \tag{1}$$

Multiplying both sides of (1) by $Y_{LM}(\hat{K})$ and integrating over $d\Omega_K$ we get

$$4\pi i^L j_L(Kr_{12})\, Y_{LM}(\hat{r}_{12}) = \int Y_{LM}(\hat{K})\, e^{i\boldsymbol{K}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)} d\Omega_K. \tag{2}$$

Using similar expansions as in (1) for $e^{iK\cdot r_1}$ and $e^{-iK\cdot r_2}$ we get

$$\text{R.H.S. of (2)} = (4\pi)^2 \sum_{l_1 m_1} \sum_{l_2 m_2} i^{l_1} (-i)^{l_2}\, j_{l_1}(Kr)\, j_{l_2}(Kr_2)\, Y_{l_1 m_1}(\hat{r}_1)$$

$$\times\, Y_{l_2 m_2}(\hat{r}_2) \int Y^{*}_{l_1 m_1}(\hat{K})\, Y^{*}_{l_2 m_2}(\hat{K})\, Y_{LM}(\hat{K})\, d\Omega_K . \tag{3}$$

The angular integration in (3) can be expressed [12] in terms of the Wigner $3j$ symbols. Thus eq. (2) becomes

$$i^L j_L(Kr_{12})\, Y_{LM}(\hat{r}_{12}) = 4\pi \sum_{l_1 m_1} \sum_{l_2 m_2} i^{l_1} (-i)^{l_2}\, j_{l_1}(Kr_1)\, j_{l_2}(Kr_2)\, Y_{l_1 m_1}(\hat{r}_1)$$

$$\times\, Y_{l_2 m_2}(\hat{r}_2)\, C(l_1, l_2, L, m_1, m_2) \begin{pmatrix} l_1 & l_2 & L \\ -m_1 & -m_2 & M \end{pmatrix} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix}, \tag{4}$$

where $C(l_1, l_2, L, m_1, m_2)$ is a multiplying factor.

From the well known properties of the $3j$ symbols we have

$$l_1 + l_2 \geq L \tag{5}$$

and

$$m_1 + m_2 = M,$$

where l_1 and l_2 are either zero or positive integers and $-l_i \leq m_i \leq l_i$ with $i = 1.2$. Now the L.H.S. of the eq. (4) contains a single spherical Bessel function of argument Kr_{12} while its R.H.S. involves product of spherical Bessel functions with arguments Kr_1 and Kr_2. Using the series expansion [13]

$$j_l(Kr) = \frac{\sqrt{\pi}}{2} \sum_{s=0}^{\infty} \frac{(-1)^s\, (Kr/2)^{l+2s}}{s!\, \Gamma(l+s+3/2)} \tag{6}$$

for all those Bessel functions in (4) we find that the lowest power of K on the L.H.S. is L and this power of K will come from the various terms of the summations on the R.H.S. satisfying the relation

$$l_1 + l_2 + 2(u + v) = L \tag{7}$$

where u and v coming from the series expansions of j_l's on the R.H.S. of (4) can have values zero or positive integers only. Eq. (7) clearly implies that

$$L \geq l_1 + l_2. \tag{8}$$

The inequalities (5) and (8) can be valid simultaneously if and only if

$$l_1 + l_2 = L. \tag{9}$$

This is the crucial point of our approach. The two double infinite summation over l_1m_1 and l_2m_2 in (4) is therefore reduced to just one *double but finite* summation over l_1m_1 (say) with l_1 varying from 0 to L and $l_2 = L - l_1$. We then equate the coefficients of K^L from both sides of (4), noting that only $u = v = 0$ terms need to be considered to obtain

$$4\pi i^L r_{12}^L Y_{LM}(\hat{r}_{12}) \frac{\pi}{2^{L+1}\Gamma(L+3/2)} = (4\pi)^2 i^L \sum_{l_1m_1} (-1)^{l_2} r_1^{l_1} Y_{l_1m_1}(\hat{r}_1)$$

$$\times r_2^{l_2} Y_{l_2m_2}(\hat{r}_2) \frac{\sqrt{\pi}}{2^{l_1+1}\Gamma(l_1+3/2)} \frac{\sqrt{\pi}}{2^{l_2+1}\Gamma(l_2+3/2)}$$

$$\times C(l_1,l_2,L,m_1,m_2) \begin{pmatrix} l_1 & l_2 & L \\ -m_1 & -m_2 & M \end{pmatrix} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} \tag{10}$$

Under the condition (9), the $3j$ symbols in (10) now get much simplified. The factor $C(l_1, l_2, L, m_1, m_2)$ and the $3j$ symbols are then obtained by comparing eqs. (107.14), (106.17) and (106.18) of reference [12] as

$$C(l_1,l_2,L,m_1,m_2) = (-1)^{m_1+m_2} (i)^{L-l_1-l_2} \left[\frac{(2L+1)(2l_1+1)(2l_2+1)}{4\pi}\right]^{1/2}, \tag{11a}$$

$$\begin{pmatrix} l_1 & l_2 & L \\ -m_1 & -m_2 & M \end{pmatrix} = (-1)^{l_1-l_2+m_1+m_2} \left[\frac{(2l_1)!\,(2l_2)!\,(L+M)!\,(L-M)!}{(2L+1)!\,(l_1+m_1)!\,(l_1-m_1)!\,(l_2+m_2)!\,(l_2-m_2)!}\right]^{1/2} \tag{11b}$$

and

$$\begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} = (-1)^L \left[\frac{(2l_1)!\,(2l_2)!}{(2L+1)!}\right]^{1/2} \frac{L!}{l_1!\,l_2!}. \tag{11c}$$

Substituting (11a)–(11c) in (10) and using the relation [14]

$$\Gamma(2z) = (2\pi)^{-1/2}\, 2^{2z-1/2}\, \Gamma(z)\, \Gamma(z + 1/2),$$

we finally get

$$r_{12}^{L}\, Y_{LM}(\hat{r}_{12}) =$$

$$\sum_{l_1 m_1}\left[\frac{4\pi\,(2L+1)\,(L+M)!\,(L-M)!}{(2l_1+1)\,(2l_2+1)\,(l_1+m_1)!\,(l_1-m_1)!\,(l_2+m_2)!\,(l_2-m_2)!}\right]^{1/2}$$

$$\times\,(-1)^{l_2}\, r_1^{l_1}\, Y_{l_1 m_1}(\hat{r}_1)\, r_2^{l_2}\, Y_{l_2 m_2}(\hat{r}_2), \tag{12}$$

where

$$l_2 = L - l_1,\; m_2 = M - m_1.$$

Eq. (12) is the required addition theorem for the regular solid harmonics.

Here we would like to mention that our approach is very similar to that of Seaton [3] only upto the eq. (3) of this article and after that his analysis is quite different.

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